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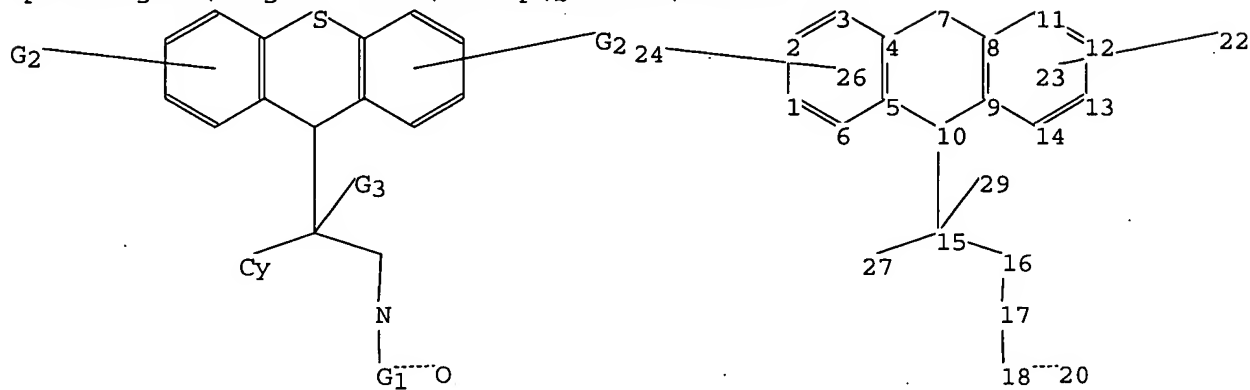
* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:49:31 ON 04 AUG 2005

=> file req

 \Rightarrow

Uploading C:\Program Files\Stnexp\Queries\10690341.str



chain nodes :

16 17 18 20 22 24 27

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

ring/chain nodes :

15 29

chain bonds :

15-16 15-27 16-17 17-18 18-20

ring/chain bonds :

10-15 15-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13
13-14

exact/norm bonds :

4-7 5-10 7-8 9-10 10-15 15-27 15-29 16-17 17-18 18-20

exact bonds :

15-16

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-11 9-14 11-12 12-13 13-14

G1 : C, S

G2: C, O, S, N, X

G3 : H, CH₂

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

```
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS
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20:CLASS  22:CLASS  23:CLASS  24:CLASS  26:CLASS  27:Atom  29:CLASS
```

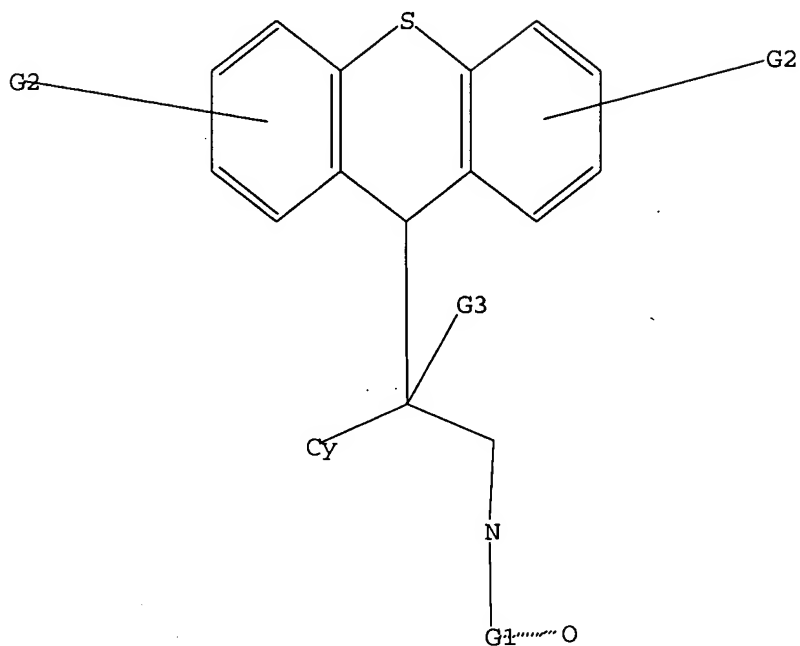
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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,S

G2 C,O,S,N,X

G3 H,CH2

Structure attributes must be viewed using STN Express query preparation.

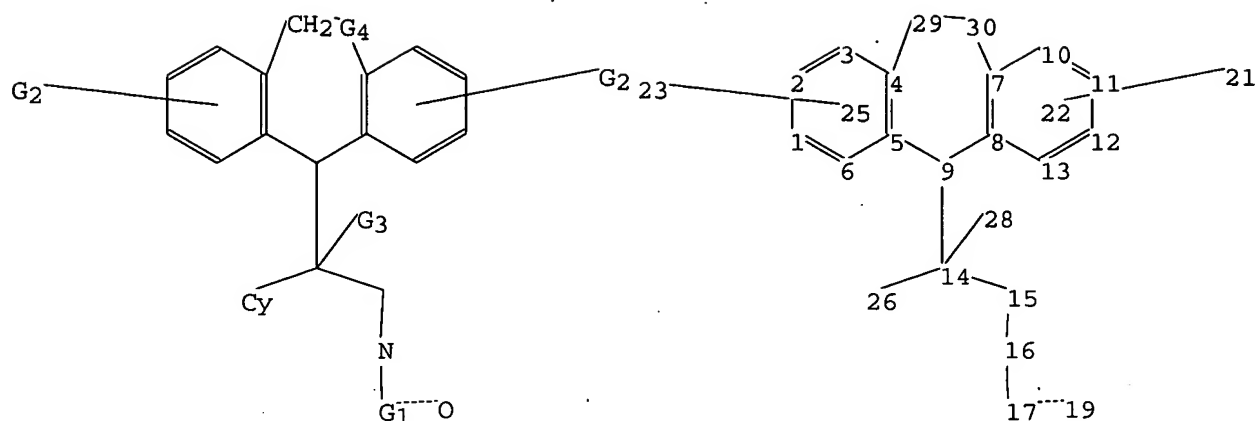
=> s l1 full

L3 0 SEA SSS FUL L1

=>

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chain nodes :

15 16 17 19 21 23 26

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 29 30

ring/chain nodes :

14 28

chain bonds :

14-15 14-26 15-16 16-17 17-19

ring/chain bonds :

9-14 14-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-29 5-6 5-9 7-10 7-8 7-30 8-9 8-13 10-11 11-12
12-13 29-30

exact/norm bonds :

4-29 5-9 7-30 8-9 9-14 14-15 14-26 14-28 15-16 16-17 17-19 29-30

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-10 7-8 8-13 10-11 11-12 12-13

G1:C,S

G2:C,O,S,N,X

G3:H,CH2

G4:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS
21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:Atom 28:CLASS 29:Atom 30:Atom

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=> d 14

L4 HAS NO ANSWERS

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

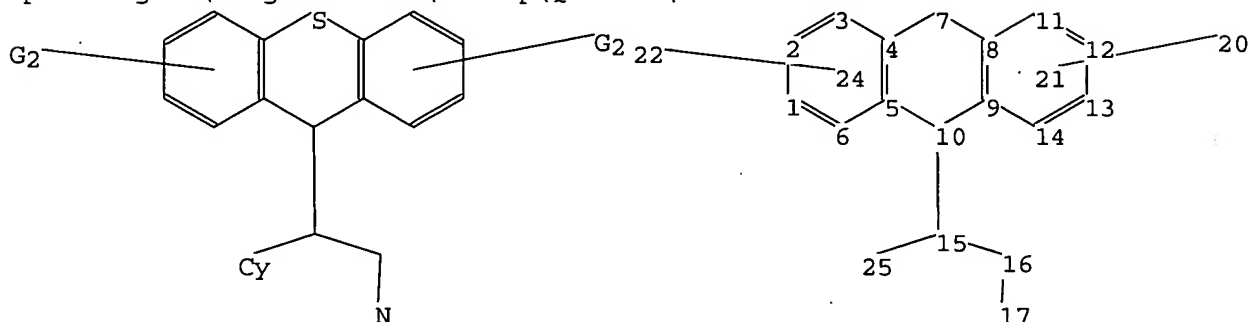
Structure attributes must be viewed using STN Express query preparation.

=> s 14 full

L6 0 SEA SSS FUL L4

=>

Uploading C:\Program Files\Stnexp\Queries\20690341.str



chain nodes :

16 17 20 22 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

ring/chain nodes :

15

chain bonds :

15-16 15-25 16-17

ring/chain bonds :

10-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14

exact/norm bonds :

4-7 5-10 7-8 9-10 10-15 15-25 16-17

exact bonds :

15-16

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-11 9-14 11-12 12-13 13-14

G1:C,S

G2:C,O,S,N,X

G3:H,CH2

Match level :

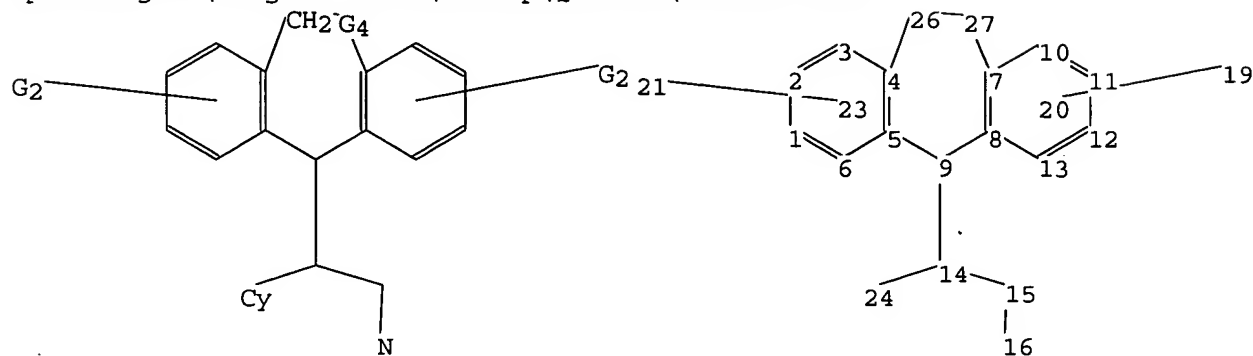
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 20:CLASS
21:CLASS 22:CLASS 24:CLASS 25:Atom

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L7 STRUCTURE UPLOADED

=>

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chain nodes :

15 16 19 21 24

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 26 27

ring/chain nodes :

14

chain bonds :

14-15 14-24 15-16

ring/chain bonds :

9-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-26 5-6 5-9 7-10 7-8 7-27 8-9 8-13 10-11 11-12

12-13 26-27

exact/norm bonds :

4-26 5-9 7-27 8-9 9-14 14-15 14-24 15-16 26-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-10 7-8 8-13 10-11 11-12 12-13

G1:C,S

G2:C,O,S,N,X

G3:H,CH2

G4:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 19:CLASS 20:CLASS

21:CLASS 23:CLASS 24:Atom 26:Atom 27:Atom

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L8 STRUCTURE UPLOADED

=> s 17 or 18 full

L10 0 SEA SSS FUL L7 OR L8

=> file marpat

=> s 110 full

STRUCTURE LOGIC NOT ALLOWED IN A DOCUMENT-BASED STRUCTURE FILE

=> s 17 full

RC BOND NOT ALLOWED IN A GENERIC STRUCTURE FILE

Searching a Markush structure file requires that all bonds in a query structure have definite specifications as ring bonds or chain bonds. The bond type 'RC', representing Ring or Chain, is not allowed for searching a Markush structure file. You may respecify the 'RC' bond in the structure as 'R' or 'C' by using the STRUCTURE command to RECALL this structure and then using the BOND command at the colon prompt (:). For more information on using these commands, enter "STRUCTURE" at an arrow prompt (=>) and then at the colon prompt (:) enter "HELP RECALL" or "HELP BOND".

=> d his

(FILE 'HOME' ENTERED AT 11:49:31 ON 04 AUG 2005)

FILE 'REGISTRY' ENTERED AT 11:49:35 ON 04 AUG 2005

L1 STRUCTURE UPLOADED

L2 0 S L1 SAM

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4 SAM

L6 0 S L4 FULL

L7 STRUCTURE UPLOADED

L8 STRUCTURE UPLOADED

L9 0 S L7 OR L8

L10 0 S L7 OR L8 FULL

FILE 'MARPAT' ENTERED AT 11:52:54 ON 04 AUG 2005

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

STN INTERNATIONAL LOGOFF AT 11:53:35 ON 04 AUG 2005